UDK 680.179:681.513

A.S. Tonkoshkur, E.L. Povzlo

DATA PROCESSING ALGORITHM OF THE GAS SENSOR RESPONSE BASED ON THE STRETCHED-EXPONENTIAL FUNCTION MODEL

Annotation. The evaluation of the suitability of the algorithm based on the model of stretched exponential function for handling the response kinetics data resistive gas sensors was carried out. This corresponds to the task of expanding the functional properties of relevant information and measurement technologies and practical application. Approbation of the algorithm on gas sensors samples based on zinc oxide ceramics has shown the efficiency for kinetics modeling of the response, after the cessation of exposure of the detected gas (methane). The next parameters were determined: static response value; average relaxation time and their distribution.

Key words: algorithm, stretched exponential function, resistive gas sensor, kinetics, response.

Introduction. The resistive gas sensors based on semiconductors are widely applied for detecting of different gases [1]. When they are used and are studied, the dependencies of static gas sensitivity (response) on the concentration of detected gas in atmosphere and temperature [2], as a rule, are used as the main functional characteristics. One of the direction, receiving the additional information about physical and chemical processes, responsible for the gas sensitivity properties of this sensor class is research of the kinetics of detection process.

It will be noted that until present, the kinetic characteristics were intended, in the main, for technical purposes, and in particular for experimental evaluation and demonstration of fast-action of the sensor elements [3-5]. Applying of modern information-measuring devices significantly increased the efficiency of the experimental researches of the considered effects on the stage of receiving and storage of the big data arrays in digital view [6]. However, at the subsequent stages of their analysis, the developments of relevant algorithms of data processing is required, which, on the one hand, would provide data on the physical parameters characterizing the kinetics of gas-sensitivity properties of the considered objects, and, on the other hand, created a base for further automation of the measurement process.

Promising theoretical basis for this purposes, is represented by using of the general phenomenological models, based on a stretched-exponential function Kohlrausch-Williams-Watts [7-8] to describe the kinetics of the relaxation dependencies of the response, particularly in the reduction step. Its feature is suitability to describe the relaxation phenomena in disordered systems in which dynamic processes occur simultaneously in many time frames [9].

Problem statement. The object of the investigation was to determine a suitability level of the algorithm, based on a stretched-exponential function for data processing of kinetic response of the resistive gas sensors.

Main part. The reaction (response) of the sensor was being determined as $S = (\sigma - \sigma_0)/\sigma_0$, where σ and σ_0 - electrical conductivity of the sensor sample in the presence and absence of detectable gas in the air. At kinetics measurements, the schema with outputs of the conductivity meter (digital electrometer) and temperature meter (thermocouple) via a matching digital device have been conjugated with computer, was implemented [6].

Time marking t produced by means of a computer. The time interval between detection of two consecutive measurements of magnitude S amounts to 0.5 seconds. The values of electrical conductivity and time are recorded in a file in computer memory during the experiment.

An example of a typical kinetic dependence on the response of the resistive gas sensor to impulse action of the active gas is represented in Fig. 1.

As previously indicated, the stretched exponential function Kohlrausch-Williams-Watts intended to approximate the relaxation kinetics of systems to their equilibrium values, i.e. to recovery processes of the sensor initial state after the cessation of exposure of the detected gas $S\left(t^{(rec)}\right)$ in the present case (Fig. 1).

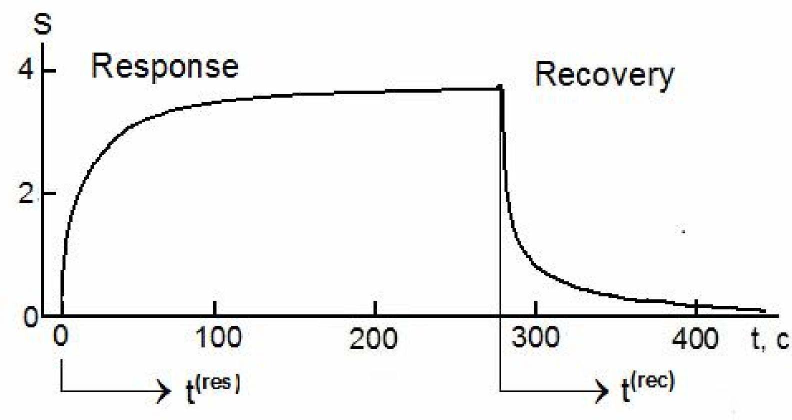


Fig 1. – Typical experimental kinetic dependence of the gas sensor sample response ($t^{(res)}$ and $t^{(rec)}$ – time axis in correspondence to detection and recovery processes)

At further description of the model will take $t = t^{(rec)}$. Stretched-exponential function [10] in this case it can be written as follows

$$S(t) = S(0) \cdot f_{KWW}(t) = S(0) \cdot \exp\left[-(t/\tau_{KWW})^{\beta}\right]. \qquad (1)$$

In (1) $S(0)$ - stationary (maximum) response value $S(t)$ at $t = 0$. Parameter τ_{KWW} is the characteristic time associated with the average relaxation time by means of the following equation [10-11]

$$t_{rel} = \int_0^{\infty} f_{KWW}(t)dt = \frac{\tau_{KWW}}{\beta}\Gamma\left(\frac{1}{\beta}\right), \qquad (2)$$

where $\Gamma(x)$ – gamma function.

Magnitude β - index, indicating the degree of tension function $f_{KWW}(t)$, which according to its representation in the form of [10,12]

$$f_{KWW}(t) = \exp\left[-(t/\tau_{KWW})^{\beta}\right] = \int_0^{\infty} z(\tau, \beta) \cdot \exp(-t/\tau) \cdot d\tau, \qquad (3)$$

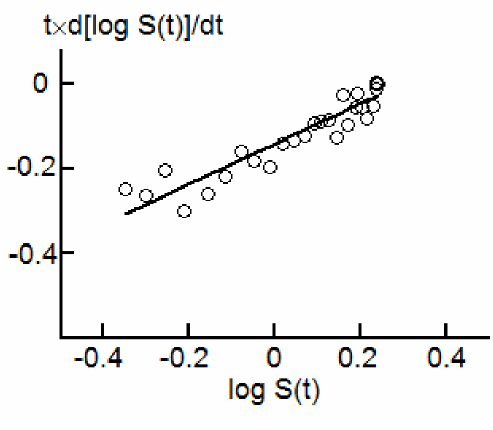
where $z(\tau, \beta)$ – the density distribution of the simple exponential relaxation processes $\exp(-t/\tau)$, linear superposition which leads to consideration stretched exponential function.

Algorithm of processing of the experimental dependences $S(t)$ on the basis of the specified model includes the following operations.

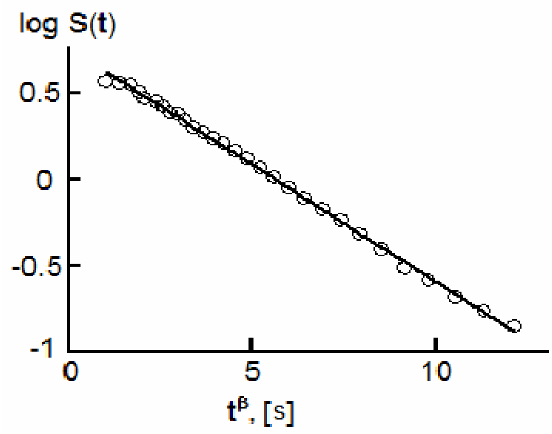
1. Primary (preliminary) data processing: counts of an electrical conductivity and time which were brought in memory of the computer in the course of the experiment are presented in the form of table dependences $\log(S_k)$ from $\log(t_k)$, where

$k = 1, 2, \dots K$. The number of counting is the magnitude of several hundred and more points of table dependence that allows carrying out their preliminary statistical processing by creation of empirical-formula regression dependence. All range of values $\log(t_k)$ was divided into n elementary segments. For each i - th elementary segment the arithmetic average $\overline{\log(S)}_i$ was calculated, to which was put the coordinate of the middle of the specified segment $\overline{\log(t)}_i$ in compliance.

2. Finding of magnitude of unknown coefficient β with use of coordinates $t \times [d \log S(t)/dt]$ and $\log S(t)$ for expression (1), in which initial dependence is straightened [12, 13] (Fig. 2a), and the coefficient is a tangent of angle of its inclination $\beta = \Delta\{\, t \times [d \log S(t)/dt]\,\}/\Delta \log S(t)$. To calculate the derivatives the initial table dependence was pre interpolated with applying of cubic splines.



a



b

Fig – 2. Dependence of the relaxation of a resistive gas sensor response after the termination of exposing of the detected gas in the coordinates used for determination of parameters β (*a*) and τ_{KWW} (*b*). Experiment – circles, the approximation by the stretched power function – solid line.

3. Determination of unknown parameters τ_{KWW} and $S(0)$ by submission of the experimental data in coordinates $\ln S(t)$ and $(t)^{\beta}$. Magnitude β – is already known. The approximating dependence is also representable by a straight line [12, 13] (Fig. 2b) and, thus, $\tau_{KWW} = \left[-\Delta \ln S(t)/\Delta(t^{\beta})\right]^{-1/\beta}$ and $S(0) = \exp\left\{\ln S(t) + (t/\tau_{KWW})^{\beta}\right\}$.

4. Calculation of average relaxation time in accordance to (2)

Results of approbation of the considered algorithm are given on Fig. 3, where the considered dependence in natural coordinates is presented $S(t)$ and t. As seen, the experimental data are well submitted by direct lines in the accepted coordinates. The relative accuracy of approximation (variation factor) of the experimental dependences expression (1) $S(t)$ is the magnitude less than 3 %.

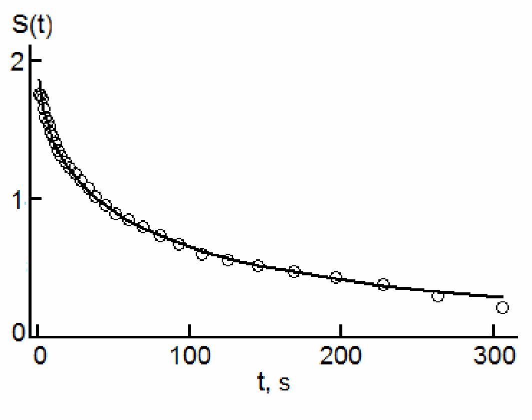


Fig – 3. Relaxation response curve of the gas sensor sample at recovering its initial state. Experiment – circles, the approximation by the stretched power function – solid line

The received values of parameters: static (maximal) value of a response $S(0)$=2.5; average relaxation time t_{rel}=150 s and the index characterizing width of distribution of the elementary exponential relaxational processes β = 0,47 are correspond to the known concepts of transition phenomena of the considered type [3-5].

Conclusions

1. Applicability of the stretched exponential function for modeling of the kinetics of the resistive gas sensors response at a recovering stage of their initial state was proved.

2. The efficiency of the given response kinetics data processing algorithm for calculation of its parameters was shown, which can be used for construction of measuring - informational technologies in the experimental researches and applying of the considered sensors.

ISSN 1562-9945

References

1. Obvintseva L.A. Metal oxide semiconductor sensors for determination of reactive gas impurities in air // Russian Journal of General Chemistry. – 2008. – 78’(12). – P.2545-2555.
2. Kupriyanov L.Y. (ed.). Semiconductor Sensors in Physic-Chemical Studies (Vol. 4): Translated from Russian by V. Yu. Vetrov. – Elsevier, 1996. – 400 p.
3. Korotcenkov G., Brinzari V., Golovanov V. & Blinov Y. Kinetics of gas response to reducing gases of SnO2 films, deposited by spray pyrolysis // Sensors and Actuators B: Chemical. – 2004. – 98’(1). – P.41-45.
4. Liewhiran C. & Phanichphant S. Influence of thickness on ethanol sensing characteristics of doctor-bladed thick film from flame-made ZnO nanoparticles // Sensors. – 2007. – 7’(2). – P.185-201.
5. Prajapati C.S. & Sahay, P. P. Alcohol-sensing characteristics of spray deposited ZnO nano-particle thin films.// Sensors and Actuators B: Chemical. – 2011. – 160’(1). – P.1043-1049.
6. Lyashkov A.Yu. Electron processes in molecules of gas sensitive ceramic structures on the base of zinc oxide doped with silver. – Manuscript. Thesis for physical and mathematical science candidate’s degree on specialty 01.04.07 – solid state physics. – Ukraine, Dniepropetrovsk: Dniepropetrovsk National University, 2011. – 167 p. (in Russian).
7. Simdyankin S.I. & Mousseau N. Relationship between dynamical heterogeneities and stretched exponential relaxation // Physical Review E. – 2003. – 68’(4). – P.041110.
8. Trzmiel J., Weron K., Janczura J. & Placzek-Popko E. Properties of the relaxation time distribution underlying the Kohlrausch–Williams–Watts photoionization of the DX centers in Cd1−xMnxTe mixed crystals // Journal of Physics: Condensed Matter. – 2009. 21’(34). – P.345801.
9. Milovanov A.V., Rasmussen J.J. & Rypdal K. Stretched-exponential decay functions from a self-consistent model of dielectric relaxation // Phys. Lett. A. – 2008. – 372’(13). – P. 2148-2154.
10. Johnston D.C. Stretched exponential relaxation arising from a continuous sum of exponential decays // Physical Review B. – 2006. – 74’(18). – P.184430.

11. Hansen E.W., Gong X. and Chen Q. Compressed Exponential Response Function Arising From a Continuous Distribution of Gaussian Decays – Distribution Characteristics // Macromolecular Chemistry and Physics. – 2013. – 214’(7). – P. 844–852.
12. Khandetskyi V.S., Tonkoshkur Yu. A. Simulation data processing isothermal depolarization analysis using functions Kohlrausch-Williams-Watts / System technologies. – 2012. – 1(78). – P. 111-120.
13. Tonkoshkur Yu.A., Lyashkov A.Yu., Tonkoshkur A.S. Isothermal depolarization current in metal-oxide varistor ceramics under various polarizing fields // Journal of advanced dielectrics. – 2013. – 3’(2), P.1350016.

О.С. Тонкошкур, Є.Л. Повзло Алгоритм обробки даних кінетики відгуку резистивного газового сенсору на основі моделі розтягнутої експоненціальної функції

Анотація. Проведено оцінку придатності алгоритму на основі моделі розтягнутої експоненціальної функції для обробки даних кінетики відгуку резистивних газових сенсорів з метою розширення функціональних властивостей відповідних інформаційно-вимірювальних технологій та практичного застосування. Апробація алгоритму на зразках газових сенсорів на основі керамічного оксиду цинку показала його ефективність для моделювання кінетики спаду відгуку після впливу активного газу (метану). Визначені параметри: статичне значення відгуку; середній час релаксації та його розподіл.

***Ключові слова**: алгоритм, розтягнута експоненціальна функція, резистивний газовий сенсор, кінетика, відгук*